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Relations between structure and morphology of crystals

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S U M M A R Y

An attempt is made to find relations between crystal structure and crystal morphology on an energy basis. After an historical approach to the subject the general principles, outlined by Hartman & Perdok (1952), are treated in greater detail in chapter II. It is concluded that the morphology of a crystal is governed by chains of strong bonds, running through the structure in a limited number of directions. The energetical period of such a chain of strong bonds is called a periodic bond chain vector (P.B.C. vector). The faces of a crystal are divided into three classes:

- (a) Flat faces or F-faces, each of which is parallel to at least two P.B.C. vectors;
- (b) Stepped faces or S-faces, each of which is parallel to at least one P.B.C. vector;
- (c) Kinked faces or K-faces which are not parallel to any P.B.C. vector.

A face parallel to two or more P.B.C. vectors may be either an F-face or an S-face. Criteria are given which serve to distinguish between them.

F-faces are the most important faces; their importance increases with increasing plane energy. S-faces are of medium importance; they can be derived from the F-faces by means of an addition scheme of indices. Their importance increases with increasing zone energy; they are the more important the lower the order of the level they occupy in the addition scheme of indices. K-faces are very rare or do not occur at all.

For a number of compounds the F-, S- and K-faces are determined and the result is compared with the observed morphological order of importance (chapters III to XIV). In general the agreement is satisfactory.

An explanation is given of several details, which can not be accounted for by the law of Donnay & Harker. Among them are:

- (a) Differences between habits of isomorphous crystals. These differences can be traced back to the following causes:
 - (1) Corresponding bonds in the two crystals are of different type (NaCl and PbS in chapter X; aragonite and cerussite in chapter XII; pyrites and hauerite in chapter XIV).
 - (2) Corresponding bonds in the two crystals are of different strength (Mg and Cd in chapter III).
 - (3) Influence of impurities (barytes and celestite in chapter XIII).

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- (b) Effect of precondensation (copper in chapter III and iron in chapter IV).
- (c) Effect of shape and position of building units (compounds with naphthalene-like structures in chapter VII; aragonite in chapter XII).
- (d) Effect of building units at special positions (dibiphenylene-ethylene in chapter VIII).
- (e) Effect of solvent (alkali halides in chapter X and XI; hydroxyl-ammoniumchloride in chapter XI).

In the chapters XV to XVIII some special topics are treated. Chapter XV deals with twins. Starting from the definition of twin given by Niggli, the possible twin laws are derived. A qualitative account is given of the distribution of the twins among the various laws. Four types of genesis of twins appear to be possible and structural and energetical conditions for the formation of twins are formulated. It is concluded that twin planes are in general F-faces. An explanation is given of the differences between the habits of twins and of single individuals. A discussion of other intergrowths between two crystals of one compound leads to the conclusion that a description of intergrowths by means of a combination of twin laws has no sense from a genetical standpoint.

A discussion in chapter XVI on the factors favouring oriented overgrowth, leads to the conclusion that preferably F-faces are in contact. Modification of the habit of deposited crystals caused by epitaxis is demonstrated and in the cases of urotropine on gypsum and of olivine inclusions in diamond, an explanation is given. Then habit modification, caused by „impurities” is discussed. The conclusion is reached that habit modification must be closely related to a potential epitaxis of impurity crystals on the crystals the habit of which is modified. In this sense an explanation is afforded of the habit change of NaCl brought about by glycine.

Chapter XVII deals with the frequency distribution of the anorthic crystals among the 202 possible complexes. It is shown that a semi-quantitative account can be given of this distribution, on the basis of the ideas outlined in chapter II.

In chapter XVIII the relations between crystal structure and crystal morphology found by Niggli, by Donnay & Harker and by McLachlan are criticised. Finally it is concluded that a qualitative energetical approach to these relations gives, on the whole, better results than former quantitative geometrical approaches.